

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Cj1507

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: Cj1507

Bond precision:	C-C = 0.0056 A	Wavelength=1.54184
Cell:	a=14.0249(5)	b=17.4283(4) c=19.1994(7)
	alpha=90	beta=103.306(4) gamma=90
Temperature:	123 K	
	Calculated	Reported
Volume	4566.9(3)	4566.9(3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C53 H77 K N2	?
Sum formula	C53 H77 K N2	C106 H154 K2 N4
Mr	781.27	1562.52
Dx,g cm-3	1.136	1.136
Z	4	2
Mu (mm-1)	1.275	1.275
F000	1712.0	1712.0
F000'	1717.41	
h,k,lmax	16,20,23	16,20,23
Nref	8314	8295
Tmin,Tmax	0.765,0.847	0.639,1.000
Tmin'	0.765	

Correction method= # Reported T Limits: Tmin=0.639 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 67.992

R(reflections)= 0.0991(5954) wR2(reflections)= 0.2918(8295)

S = 1.071 Npar= 507

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

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.199
PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 0.199 Report
PLAT213_ALERT_2_B Atom C30 has ADP max/min Ratio 4.4 oblate
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 13 Note

Alert level C

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.29 Report
PLAT213_ALERT_2_C Atom C3 has ADP max/min Ratio 3.2 oblate
PLAT213_ALERT_2_C Atom C4 has ADP max/min Ratio 3.8 oblate
PLAT213_ALERT_2_C Atom C9 has ADP max/min Ratio 3.9 oblate
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.2 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of K1 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.6 Note
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00559 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 5.262 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 6 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.95A From N2 0.41 eA-3

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 2.00 Check
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT303_ALERT_2_G Full Occupancy Atom H4A with # Connections 2.00 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 40.40 Deg.
K1 -C4 -H4A 1_555 1_555 1_555 # 52 Check
PLAT793_ALERT_4_G Model has Chirality at C3 (Centro SPGR) S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints 24 Note
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 54% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.7 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info

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

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

