

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision:	C-C = 0.0036 A	Wavelength=0.71073
Cell:	a=13.5987(14)	b=10.8791(10) c=14.1825(12)
	alpha=90	beta=108.631(10) gamma=90
Temperature:	173 K	
	Calculated	Reported
Volume	1988.2(3)	1988.2(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	C26 H18 F3 N	C26 H18 F3 N
Sum formula	C26 H18 F3 N	C26 H18 F3 N
Mr	401.41	401.41
Dx, g cm ⁻³	1.341	1.341
Z	4	4
Mu (mm ⁻¹)	0.097	0.097
F000	832.0	832.0
F000'	832.46	
h, k, lmax	18, 14, 19	17, 14, 18
Nref	5458	4574
Tmin, Tmax	0.977, 0.981	0.840, 0.860
Tmin'	0.977	

Correction method= # Reported T Limits: Tmin=0.840 Tmax=0.860
AbsCorr = MULTI-SCAN

Data completeness= 0.838 Theta(max)= 29.328

R(reflections)= 0.0567(2322)	wR2(reflections)=
S = 1.014	0.1786(4574)
Npar= 271	

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	C2	--C3	.	5.5 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C6	--C7	.	7.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C7	--C8	.	6.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C19	--C26	.	5.5 s.u.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			4.449 Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).				9 Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600			11 Report



Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...				2 Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records				1 Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar			0.0200	Report
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of			C26	Check
PLAT793_ALERT_4_G	Model has Chirality at C17	(Centro SPGR)			R Verify
PLAT793_ALERT_4_G	Model has Chirality at C18	(Centro SPGR)			R Verify
PLAT793_ALERT_4_G	Model has Chirality at C19	(Centro SPGR)			S Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints			1 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary				Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600			805 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity			2.0 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				1 Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by				4 Check

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

7 ALERT type 2 Indicator that the structure model may be wrong or deficient

6 ALERT type 3 Indicator that the structure quality may be low

5 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.

