

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) bmk2255

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: bmk2255

Bond precision: C-C = 0.0043 Å Wavelength=0.71073

Cell: a=7.7175(10) b=11.1752(18) c=11.6839(15)
 alpha=73.654(13) beta=75.259(11) gamma=76.247(13)
Temperature: 293 K

	Calculated	Reported
Volume	920.0(2)	920.0(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H16 N4 O3	?
Sum formula	C22 H16 N4 O3	C22 H16 N4 O3
Mr	384.39	384.39
Dx, g cm ⁻³	1.388	1.388
Z	2	2
Mu (mm ⁻¹)	0.095	0.095
F000	400.0	400.0
F000'	400.17	
h, k, lmax	10, 15, 16	10, 14, 15
Nref	5170	4310
Tmin, Tmax	0.983, 0.992	0.460, 1.000
Tmin'	0.962	

Correction method= # Reported T Limits: Tmin=0.460 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.834 Theta(max)= 29.588

R(reflections)= 0.0635(2698)	wR2(reflections)=
S = 1.056	0.1858(4310)
Npar= 263	

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

PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	N4	Check
PLAT334_ALERT_2_C	Small	<C-C> Benzene Dist. C17 -C22 .	1.37	Ang.
PLAT340_ALERT_3_C	Low	Bond Precision on C-C Bonds	0.0043	Ang.
PLAT906_ALERT_3_C	Large	K Value in the Analysis of Variance	15.655	Check
PLAT910_ALERT_3_C	Missing	# of FCF Reflection(s) Below Theta(Min).	8	Note
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L= 0.600	3	Report
PLAT934_ALERT_3_C	Number of	(Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1	Check



Alert level G

PLAT199_ALERT_1_G	Reported	_cell_measurement_temperature	(K)	293	Check
PLAT200_ALERT_1_G	Reported	_diffrn_ambient_temperature	(K)	293	Check
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		798	Note
PLAT941_ALERT_3_G	Average	HKL Measurement Multiplicity		1.8	Low
PLAT978_ALERT_2_G	Number	C-C Bonds with Positive Residual Density.		0	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
7 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
1 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.

