

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) be12jea2n

No syntax errors found. CIF dictionary Interpreting this report

Datablock: be12jea2n

Bond precision: C-C = 0.0048 A Wavelength=0.71073

Cell: a=6.66100 b=30.08300 c=17.63500
 alpha=90 beta=99.5200 gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	3485.085	3485
Space group	P 21/n	?
Hall group	-P 2yn	?
Moiety formula	C24 H15 N O2	?
Sum formula	C24 H15 N O2	C48 H30 N2 O4
Mr	349.37	698.74
Dx, g cm ⁻³	1.332	1.332
Z	8	4
Mu (mm ⁻¹)	0.085	0.085
F000	1456.0	1456.0
F000'	1456.64	
h,k,lmax	7,35,20	7,35,20
Nref	5936	5915
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.996 Theta(max)= 24.710

R(reflections)= 0.0628(3206) wR2(reflections)= 0.1599(5915)

S = 1.034 Npar= 487

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 A

PLAT053_ALERT_1_A Minimum Crystal Dimension Missing (or Error) ...	?
PLAT054_ALERT_1_A Medium Crystal Dimension Missing (or Error) ...	?
PLAT055_ALERT_1_A Maximum Crystal Dimension Missing (or Error) ...	?
PLAT122_ALERT_1_A No _symmetry_space_group_name_H-M Given	?

Alert level B

PLAT052_ALERT_1_B Info on Absorption Correction Method Missing ... ?
PLAT093_ALERT_1_B No su's on H-atoms, but refinement reported as . mixed

Alert level C

THETM01_ALERT_3_C The value of $\sin(\theta_{\max})/\lambda$ is less than 0.590
Calculated $\sin(\theta_{\max})/\lambda = 0.5882$
PLAT045_ALERT_1_C Calculated and Reported Z Differ by 2.00 Ratio
PLAT141_ALERT_4_C su on a - Axis Small or Missing 0.00000 Ang.
PLAT142_ALERT_4_C su on b - Axis Small or Missing 0.00000 Ang.
PLAT143_ALERT_4_C su on c - Axis Small or Missing 0.00000 Ang.
PLAT145_ALERT_4_C su on beta Small or Missing 0.0000 Deg.
PLAT151_ALERT_1_C No su (esd) Given on Volume ?
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.6
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.3
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.0048 Ang

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ?
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c P21/n
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max datum ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min datum ?
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature 293 K
PLAT200_ALERT_1_G Check the Reported _diffrn_ambient_temperature 293 K

- 4 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
10 **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
- 13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
5 ALERT type 4 Improvement, methodology, query or suggestion
1 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*, 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.

PLATON version of 19/04/2012; check.def file version of 14/04/2012

Datablock be12jea2n - ellipsoid plot

