

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) AX2854abs

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: AX2854abs

Bond precision:	C-C = 0.0047 Å	Wavelength=0.71073
Cell:	a=12.0690 (15)	b=7.6497 (9) c=16.1743 (19)
	alpha=90	beta=110.812 (2) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	1395.9 (3)	1395.8 (3)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C26 H36 N6 O8	C26 H36 N6 O8
Sum formula	C26 H36 N6 O8	C26 H36 N6 O8
Mr	560.61	560.61
Dx, g cm-3	1.334	1.334
Z	2	2
Mu (mm-1)	0.100	0.100
F000	596.0	596.0
F000'	596.29	
h, k, lmax	14, 9, 19	14, 9, 19
Nref	5496 [2965]	5495
Tmin, Tmax	0.979, 0.986	0.701, 0.746
Tmin'	0.976	

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Correction method= # Reported T Limits: Tmin=0.701 Tmax=0.746
AbsCorr = MULTI-SCAN
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Data completeness= 1.85/1.00 Theta(max)= 25.999

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R(reflections)= 0.0417( 4923)      wR2(reflections)=
S = 1.022                        0.1058( 5495)
Npar= 380
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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

PLAT213_ALERT_2_B Atom C16' has ADP max/min Ratio 4.1 prolat



Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C17 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00473 Ang.



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.300 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 3% Note
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H23C ..H16F . 2.09 Ang.
1-x,-1/2+y,2-z = 2_647 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O3 ..C3 . 2.95 Ang.
1-x,1/2+y,1-z = 2_656 Check
PLAT791_ALERT_4_G Model has Chirality at C13 (Sohncke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C20 (Sohncke SpGr) S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints 3 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min) [Deg]= 1.81 Note
0 0 1,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
0 0 1,
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 52.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 5.719 Note
Predicted wR2: Based on SigI**2 1.85 or SHELX Weight 10.36
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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

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

