checkCIF/PLATON report

Structure factors have been supplied for datablock(s) test6_a

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: test6_a

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Bond precision:   C-C = 0.0150 A          Wavelength=0.71073

Cell:             a=10.537(6)     b=10.802(6)          c=15.329(8)
                  alpha=90        beta=94.978(15)      gamma=90
Temperature:      303 K
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	Calculated	Reported
Volume	1738.2(17)	1738.2(16)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C15 H27 N O4	C15 H27 N O4
Sum formula	C15 H27 N O4	C15 H27 N O4
Mr	285.38	285.37
Dx,g cm-3	1.090	1.091
Z	4	4
Mu (mm-1)	0.078	0.078
F000	624.0	624.0
F000'	624.31	
h,k,lmax	12,13,18	12,12,18
Nref	6385[3376]	5685
Tmin,Tmax	0.991,0.993	0.471,0.745
Tmin'	0.966	

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Correction method= # Reported T Limits: Tmin=0.471 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.68/0.89        Theta(max)= 25.391

R(reflections)= 0.0933( 3064)                    wR2(reflections)=
                                                 0.2079( 5685)
S = 1.045                  Npar= 374
```

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

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.015 Ang.

Alert level C

STRVA01_ALERT_4_C Flack parameter is too small
From the CIF: _refine_ls_abs_structure_Flack -0.500
From the CIF: _refine_ls_abs_structure_Flack_su 1.000

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 3.8 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range 4.7 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C5 --C6 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C17 --C18 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C19 --C20 . 0.16 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O8 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C5 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C12 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C16 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C18 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C19 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C27 Check
PLAT245_ALERT_2_C U(iso) H3 Smaller than U(eq) O3 by 0.025 Ang**2
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O5 0.106 Check
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O3 - H3 . 1.02 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 18.777 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.301 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 5.267 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.661 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.507 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.060 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 14 Report
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage 78 %

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF ..... Please Check
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 1.000 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O4 . 108.6 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O8 . 107.2 Degree
PLAT791_ALERT_4_G Model has Chirality at C3 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C4 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C18 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C19 (Sohnke SpGr) R Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 31 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 3 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.80 Check

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
25 **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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
15 ALERT type 2 Indicator that the structure model may be wrong or deficient
13 ALERT type 3 Indicator that the structure quality may be low
11 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.

PLATON version of 19/02/2022; check.def file version of 19/02/2022

Datablock test6_a - ellipsoid plot