

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) i18888

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: i18888

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Bond precision:	C-C = 0.0036 Å	Wavelength=0.71073
Cell:	a=16.4657(4) alpha=90	b=10.4086(3) beta=96.402(1) c=20.1302(6) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	3428.50(17)	3428.50(16)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C23 H28 N4, C6 H4 F N O2, 2(C4 H8 O)	C23 H28 N4, C6 H4 F N O2, 2(C4 H8 O)
Sum formula	C37 H48 F N5 O4	C37 H48 F N5 O4
Mr	645.80	645.80
Dx, g cm <sup>-3</sup>	1.251	1.251
Z	4	4
Mu (mm <sup>-1</sup> )	0.086	0.086
F000	1384.0	1384.0
F000'	1384.60	
h,k,lmax	21,13,25	21,13,25
Nref	7606	7585
Tmin,Tmax	0.978,0.987	0.919,1.000
Tmin'	0.978	

Correction method= # Reported T Limits: Tmin=0.919 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.997      Theta(max)= 27.171

R(reflections)= 0.0658( 5367)

wR2(reflections)=  
0.2045( 7585)

S = 1.030

Npar= 463

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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.

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#### Alert level C

PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.89Ang From C1 . 0.62 eA-3

**Author Response: This peak at the carbone C-atom C1 could be modeled as an H-atom which would be within H-bonding distance to O1 D-H H...A D...A <(DHA) 0.99(3) 2.50(3) 3.448(3) 160(2) C1-H1...O1 but EPR spectroscopy strongly suggests that this electron density results from a three electron radical plus lone pair (see main discussion).**

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#### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	20	Note
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.10	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	10	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2	Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 6)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 3)	8.11	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 4)	7.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 5)	4.89	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 6)	5.50	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for C1		Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O3	108.4	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O3A	105.4	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O4A	106.6	Degree
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	94	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min). -1 0 1, 1 0 1, 0 0 2,	3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	17	Note
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value ..... Predicted wR2: Based on SigI**2 3.50 or SHELX Weight 20.49	5.85	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

21 **ALERT level G** = General information/check it is not something unexpected

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

8 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

11 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* 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.

