

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) i19025

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: i19025

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Bond precision:      C-C = 0.0050 A

Wavelength=0.71073

Cell:                      a=11.5473(5)                      b=11.6164(7)                      c=15.7781(9)  
                              alpha=77.205(3)                      beta=76.299(3)                      gamma=65.367(3)  
Temperature:              100 K

	Calculated	Reported
Volume	1850.96(18)	1850.96(18)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C29 H32 N6 O4), 5(C4 H8 O)	C29 H32 N6 O4, 2.5(C4 H8 O)
Sum formula	C78 H104 N12 O13	C39 H52 N6 O6.50
Mr	1417.73	708.86
Dx, g cm <sup>-3</sup>	1.272	1.272
Z	1	2
Mu (mm <sup>-1</sup> )	0.088	0.088
F000	760.0	760.0
F000'	760.33	
h,k,lmax	13,13,18	13,13,18
Nref	6520	6516
Tmin,Tmax	0.992,0.996	0.803,0.970
Tmin'	0.989	

Correction method= # Reported T Limits: Tmin=0.803 Tmax=0.970  
AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 25.000

R(reflections)= 0.0640( 4202)

wR2(reflections)=  
0.1882( 6516)

S = 1.034

Npar= 586

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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 B

RINTA01\_ALERT\_3\_B The value of Rint is greater than 0.18  
Rint given 0.206

**Author Response: This compound consistently deposits as multiple crystals that require sectioning prior to diffraction. The data herein represent the best of several trials.**

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#### Alert level C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
	Calc: 2(C29 H32 N6 O4), 5(C4 H8 O)	
	Rep.: C29 H32 N6 O4, 2.5(C4 H8 O)	
PLAT214_ALERT_2_C	Atom C36A (Anion/Solvent) ADP max/min Ratio	4.9 oblate
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00504 Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.595	3 Report
	0 1 1, -2 0 2, 2 1 2,	
PLAT977_ALERT_2_C	Check Negative Difference Density on H37B .	-0.33 eA-3

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#### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	25 Note
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H Atoms	25 Report
PLAT020_ALERT_3_G	The Value of Rint is Greater Than 0.12 .....	0.206 Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500 Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.003 Degree
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2 Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	3 Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	5 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200 Report
PLAT300_ALERT_4_G	Atom Site Occupancy of O7 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C38 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C39 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C40 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C41 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H38A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H38B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H41A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H41B Constrained at	0.5 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100% Note
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 2)	7.96	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 3)	8.45	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 4)	6.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 5)	5.04	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 6)	4.55	Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O5	.	109.0	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O6	.	108.0	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O7	.	109.9	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O5A	.	109.6	Degree
PLAT411_ALERT_2_G	Short Inter H...H Contact H24 ..H37C	.	2.11	Ang.
	1-x,1-y,1-z =		2_666	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H22C ..H37D	.	2.11	Ang.
	1-x,1-y,1-z =		2_666	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C25 ..C37A	.	3.06	Ang.
	1-x,1-y,1-z =		2_666	Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		13	Check
PLAT793_ALERT_4_G	Model has Chirality at C24 (Centro SpGr)		S	Verify
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers		1	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		642	Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still		35%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1	Note
	0 0 1,			
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....		2	Note
	-2 0 2, 2 1 2,			
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		2	Note
	2 1 2, -2 0 2,			
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...		4	Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..		50.0	Degree
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....		3.090	Note
	Predicted wR2: Based on SigI**2 6.09 or SHELX Weight 18.21			
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		3	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  
 5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 53 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 13 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 12 ALERT type 3 Indicator that the structure quality may be low  
 29 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.

